

Intricacies of Counterflow Flames in Validating Chemical Kinetic Models

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Acknowledgements:

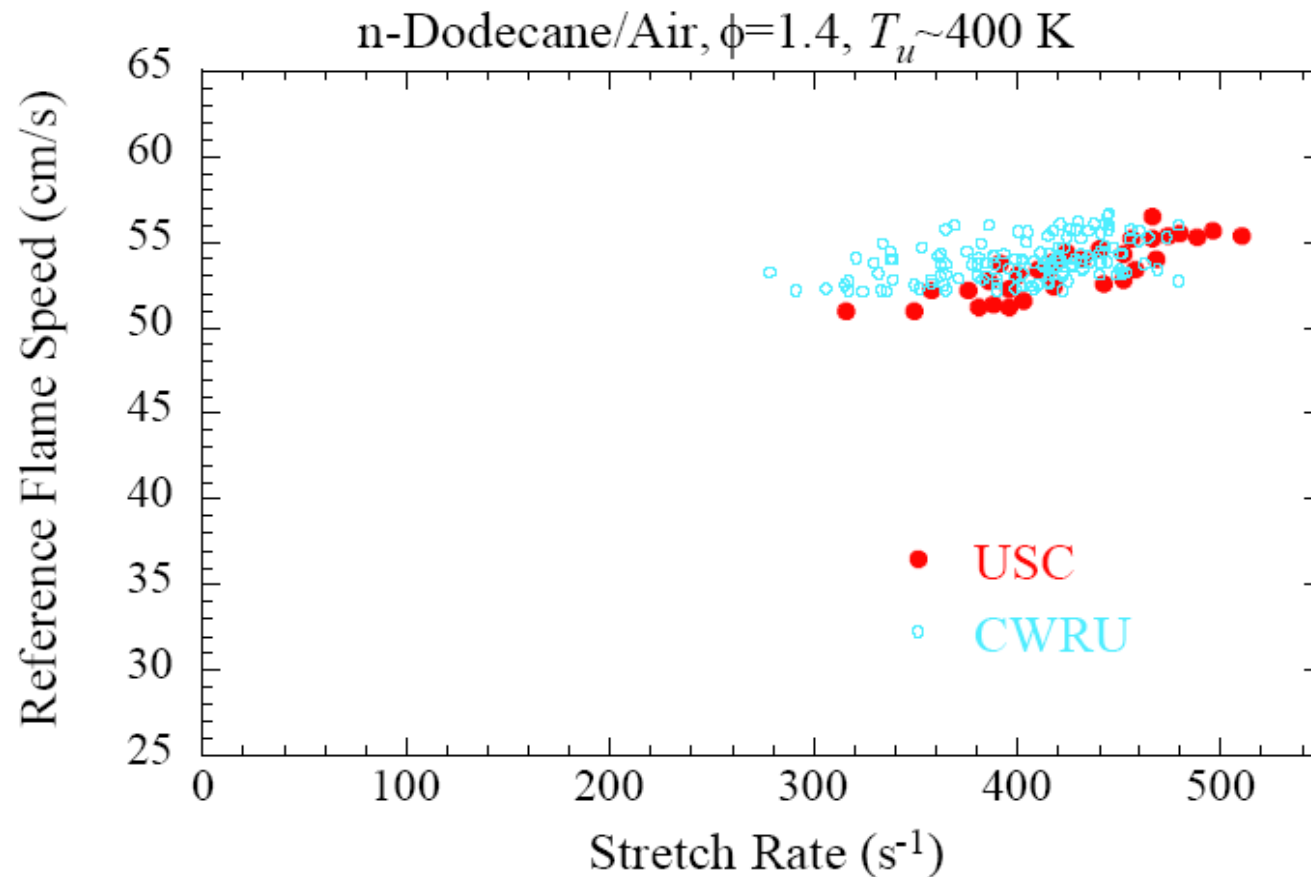
Gaetano Esposito, Brendyn Sarnacki, Vish Katta

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OSD TE & ST Program

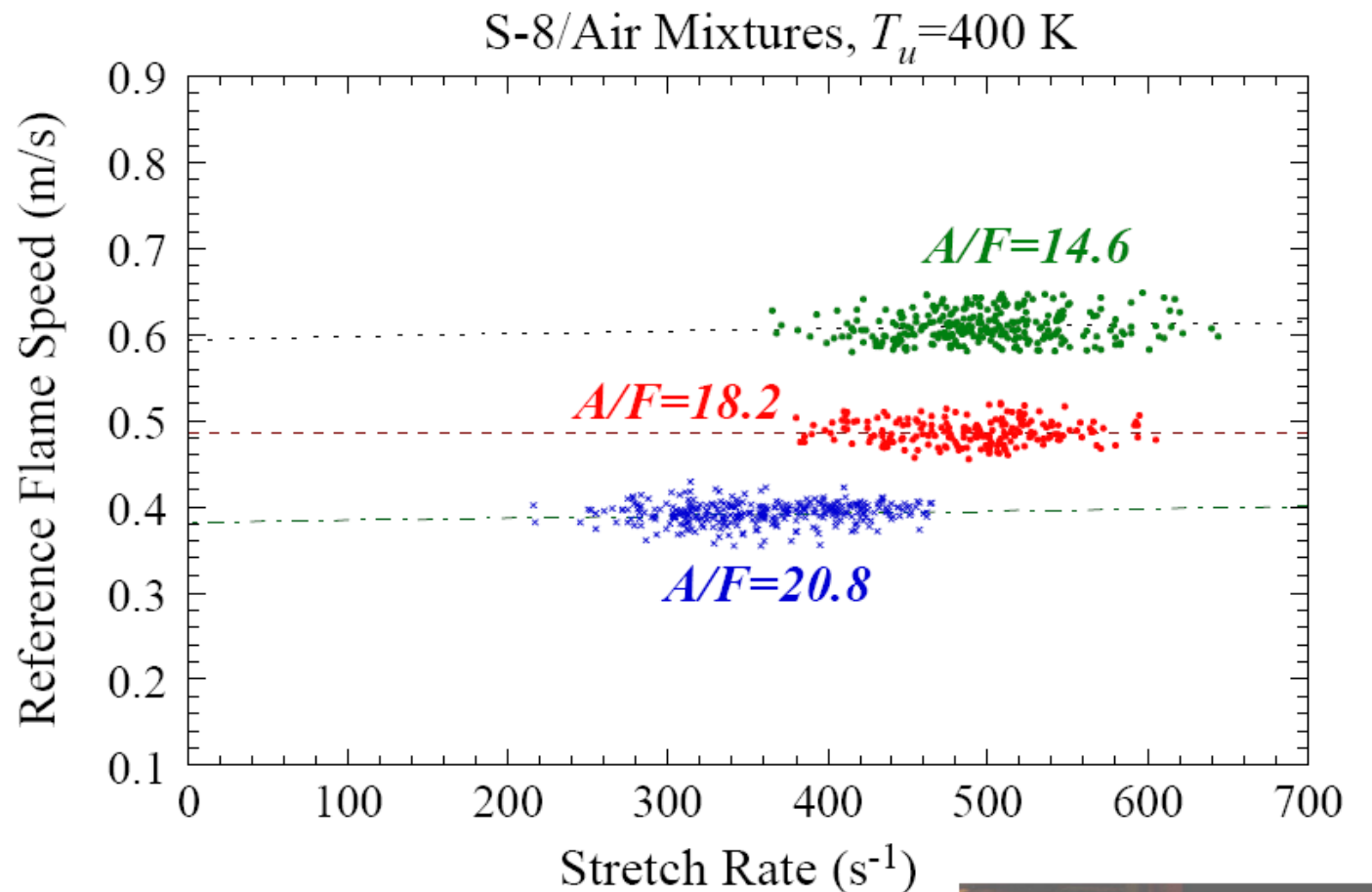
Motivation

- Experimental data presented at the last MACCCR Meeting by Jackie Sung



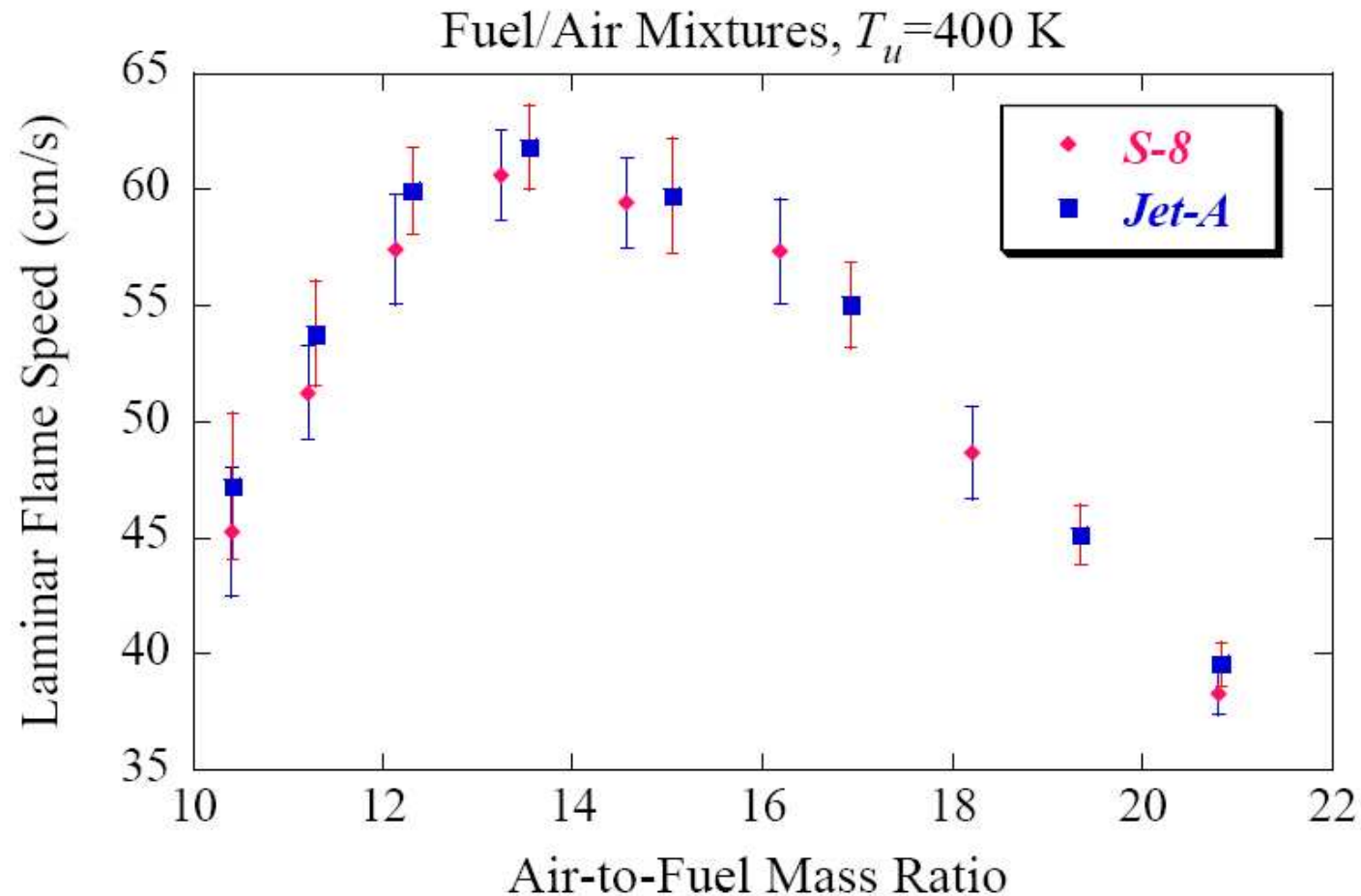
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Questions?

- How accurate is the local strain rate, reference velocity, ...?
- Can we use an alternate **counterflow flame property** for optimization and validation of chemical kinetic models?

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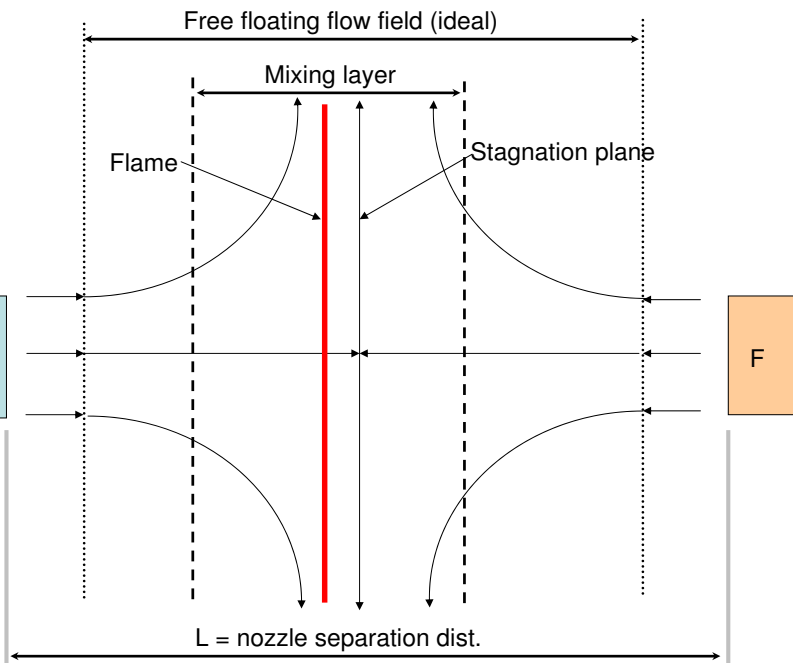
Extinction Strain Rate of Nonpremixed Flames

Outline

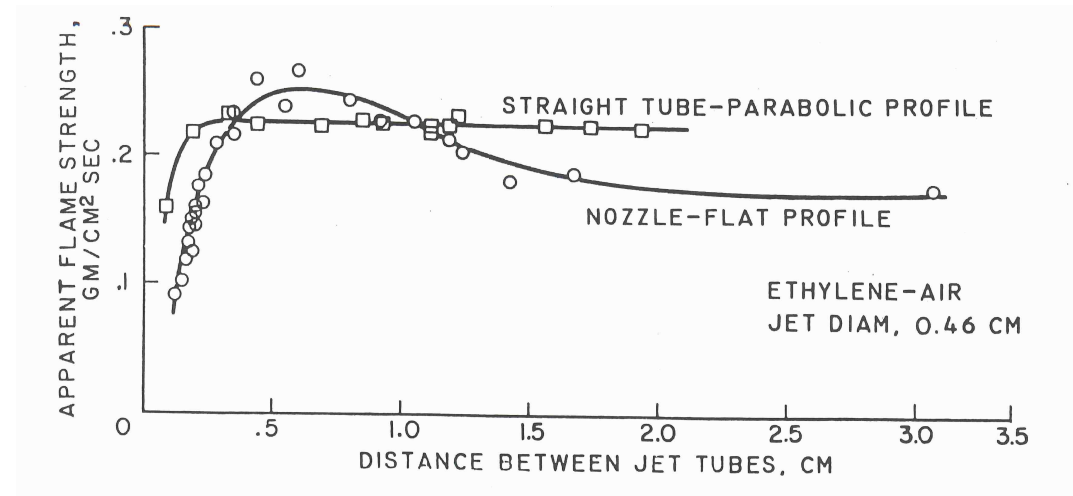
- A brief review
- Uncertainties of experimental data:
 - premixed flames (last MACCCR Fuels Meeting at NIST)
 - non-premixed flames (eg. ethylene-air data of USC, NASA Langley, and UVa)
- Two-dimensional effects?
 - LDV and PIV data
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- Concluding remarks

Review - Free-floating Limit

- Ideal, free-floating counterflow field for $L/D > 2$



Ideal case

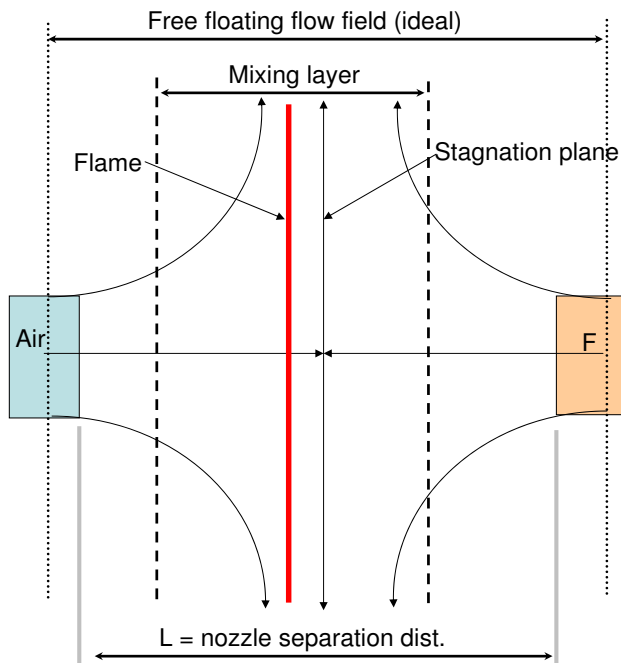


Potter, Heimel, and Buttler
Eighth Combustion Symposium, 1960

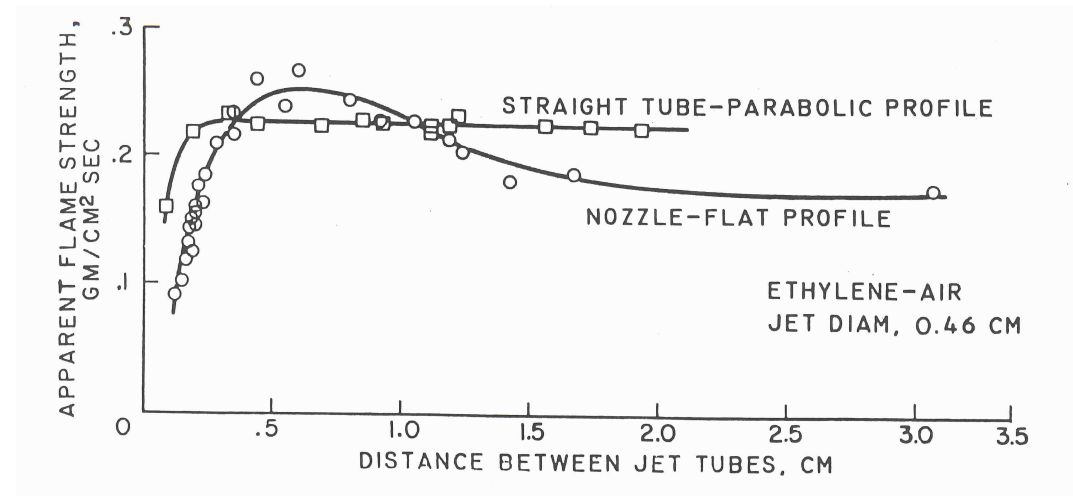
$$a_{global} \sim 1900s^{-1} \text{ at } L/D \sim 1$$

Review - Free-floating Limit

- Non-ideal counterflow field for $L/D < 1$



Non-ideal case

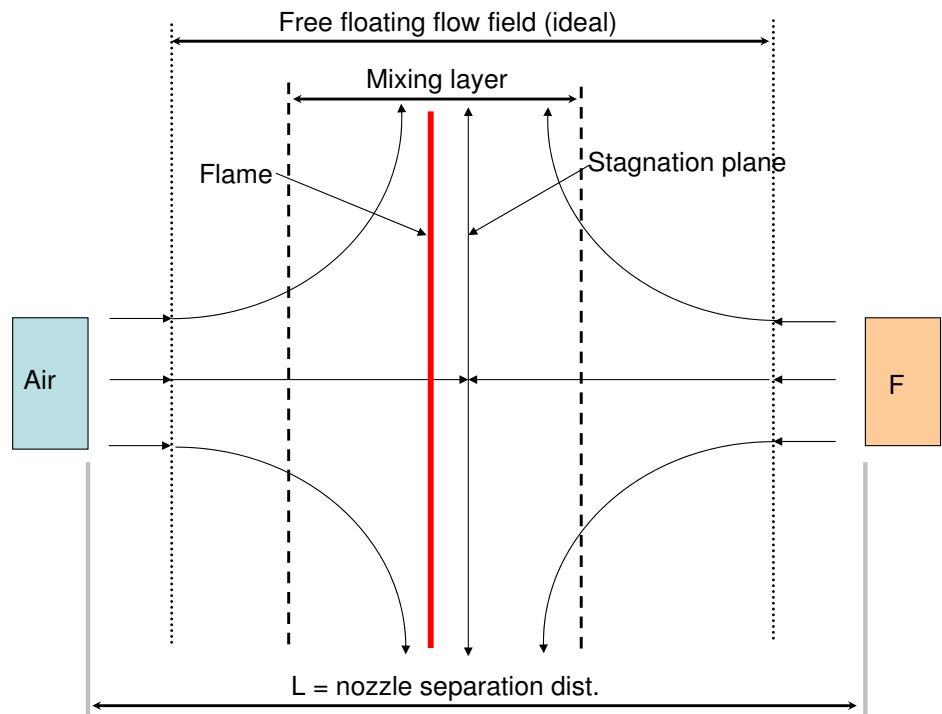
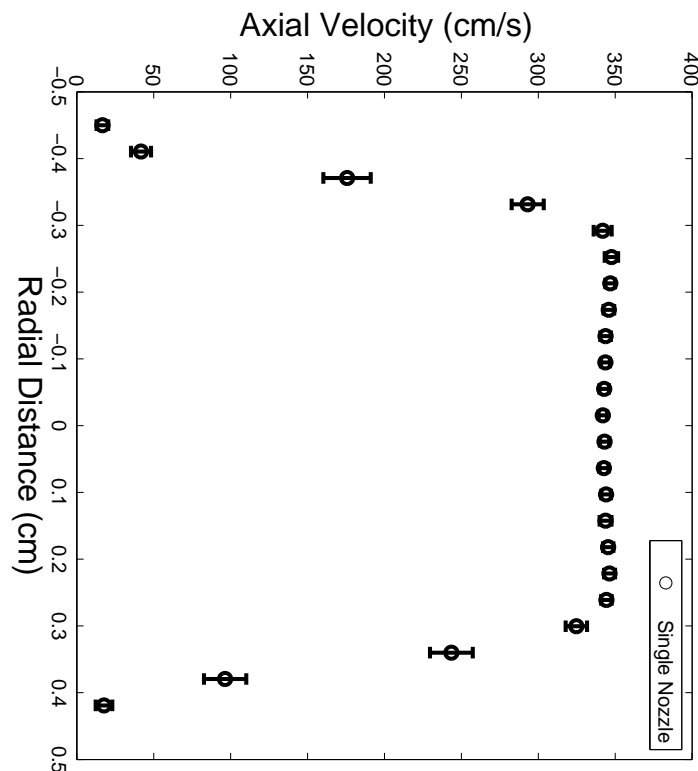


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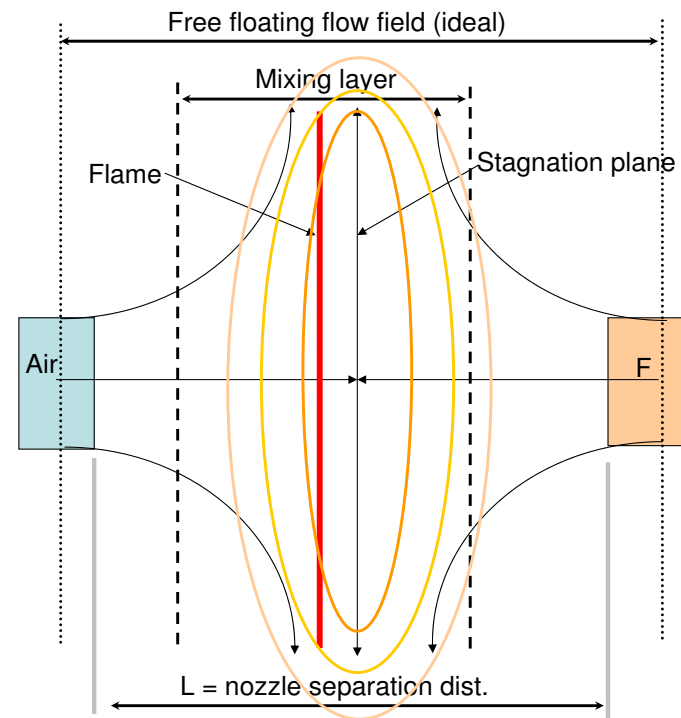
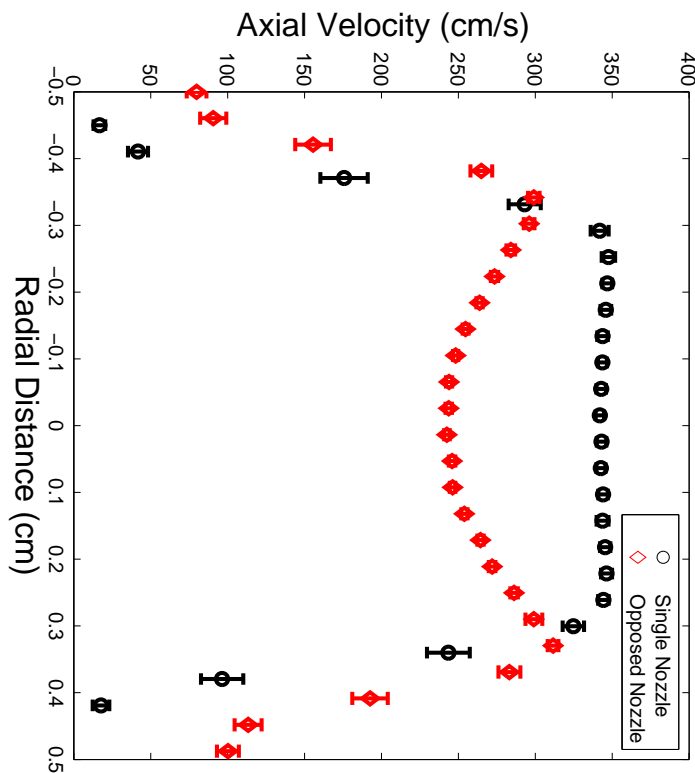
Review - Influence of Nozzle Exit Profile

- Non-ideal separation distance effect on nozzle exit velocity profile
- First demonstrated by Rolon et al. in early 1990's.



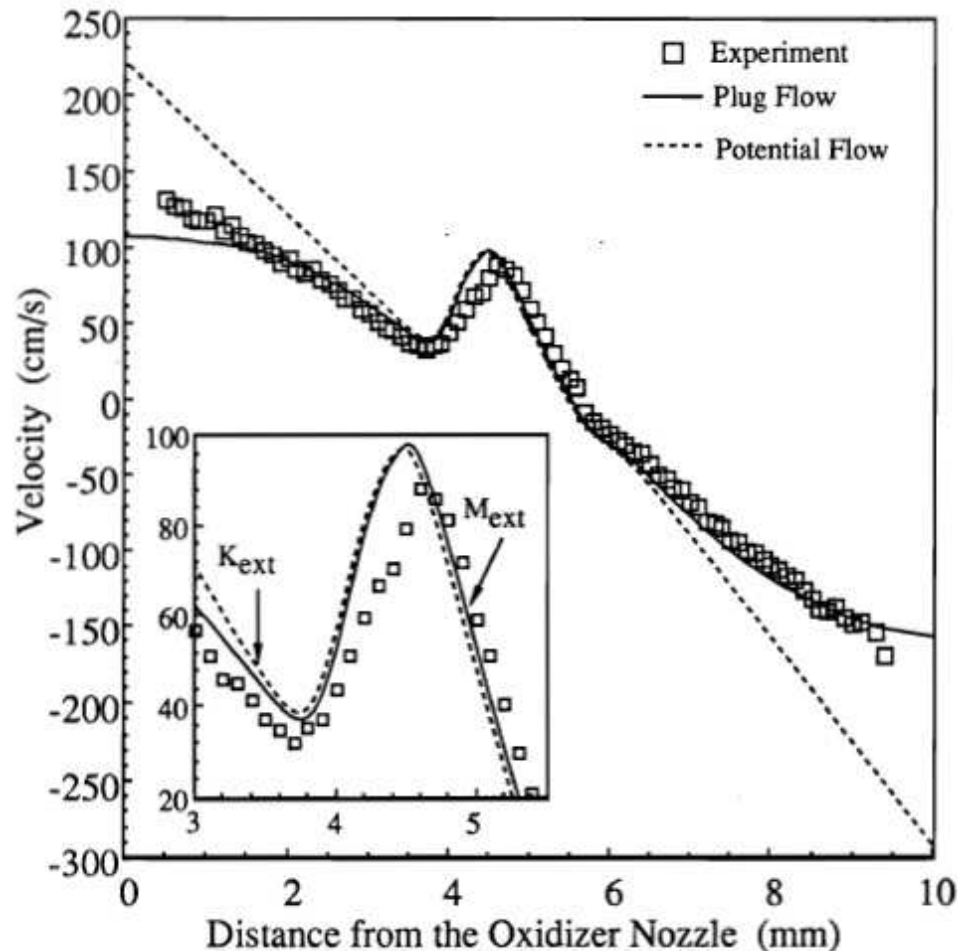
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Review - Influence of Radial Boundary Condition

- Finite $\partial v_r / \partial r (\equiv U)$ (Chelliah et al., 23rd Symp., 1990, Smooke et al. 1990)
- Axial velocity of methane-air non-premixed flames near extinction



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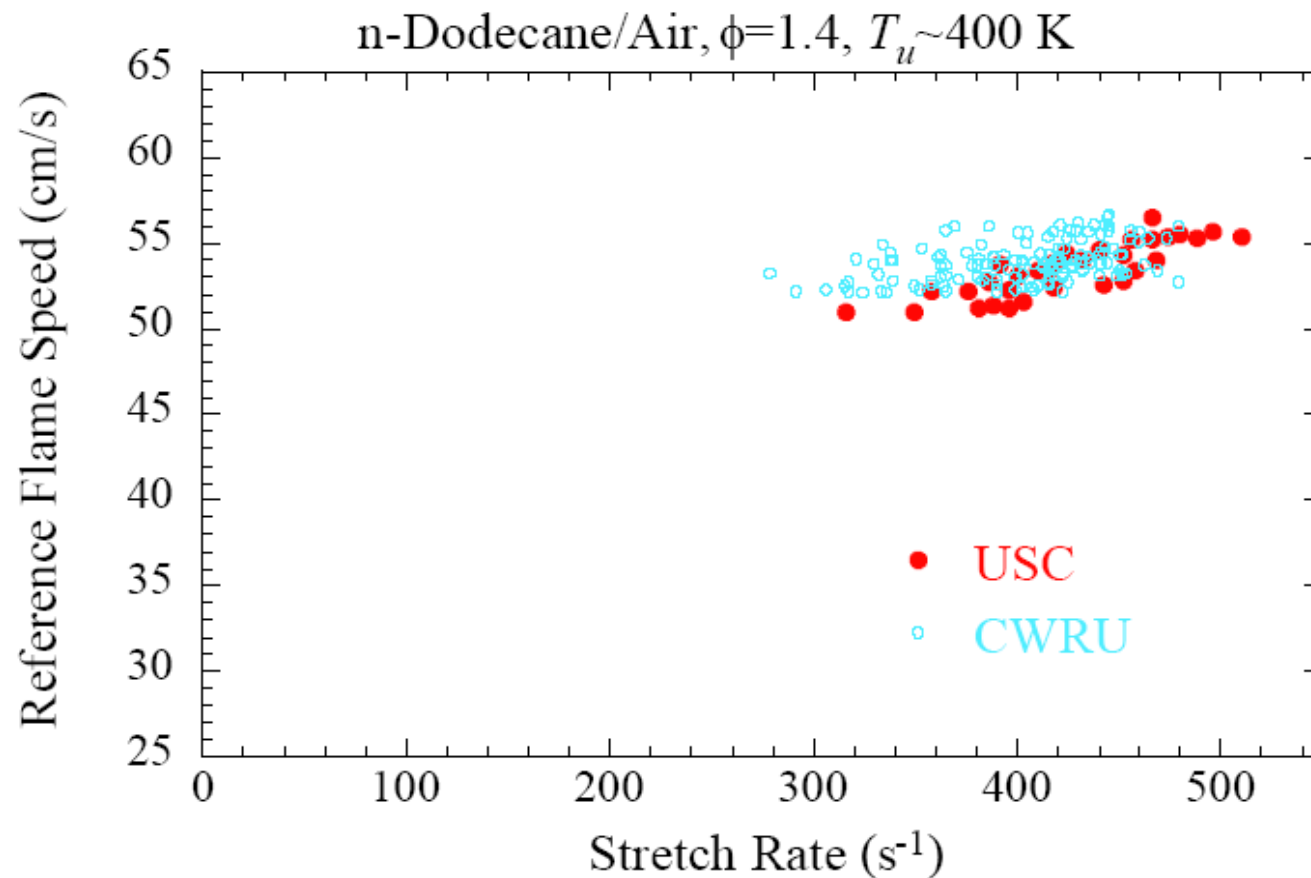
Uncertainties – Burning Velocity of Premixed Flames

- Three key uncertainties

(i) local strain rate,

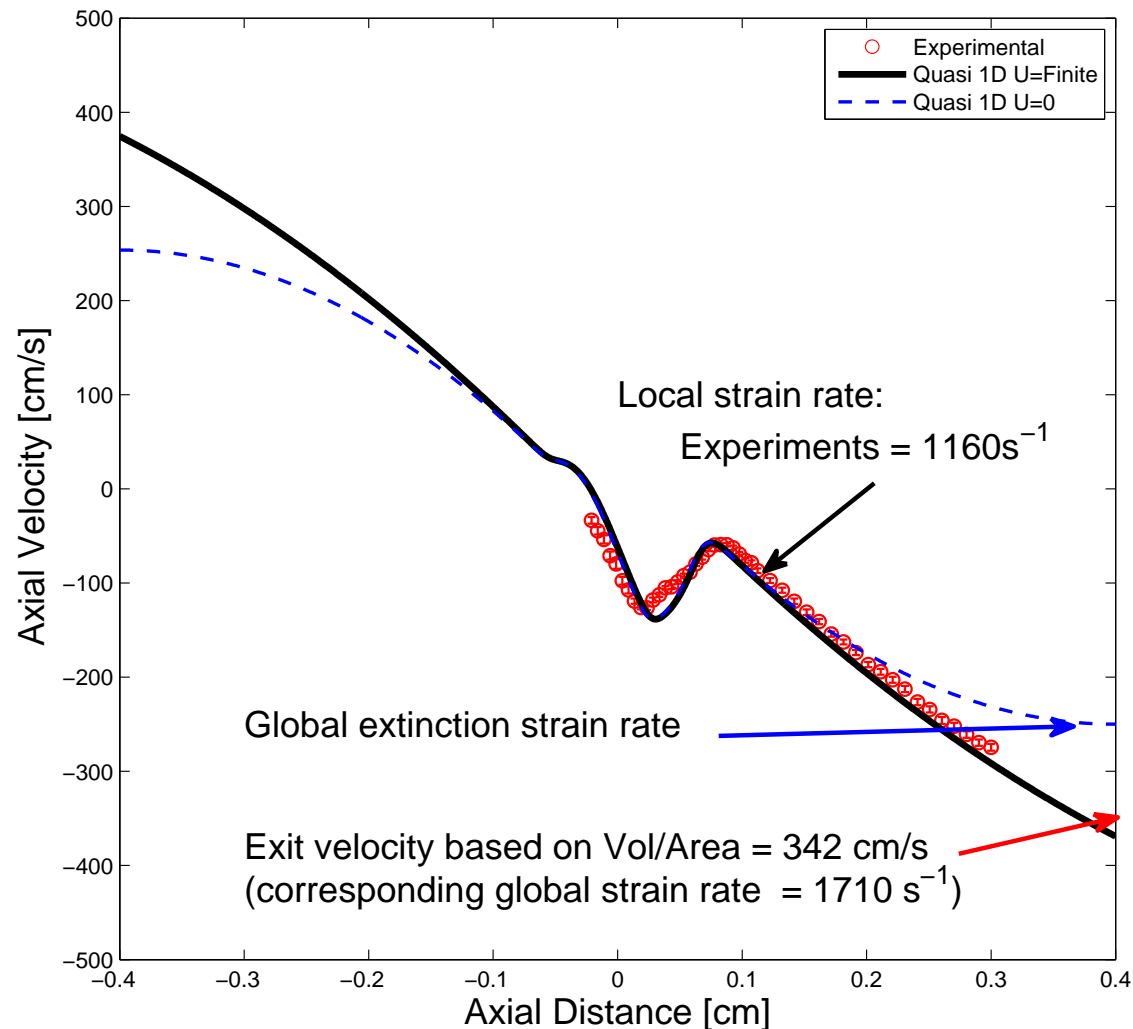
(ii) reference velocity

(ii) linear vs. non-linear extrapolation (Stahl, Warnatz, and Rogg, 1988).



Some Definitions of Nonpremixed Flame Characteristics

- Global Strain Rate $a_{global} = 4 v_{air} / L$ (Seshadri and Williams, 1978)
where v_{air} from (i) Volume/Area, (ii) LDV/PIV, and (iii) computations.



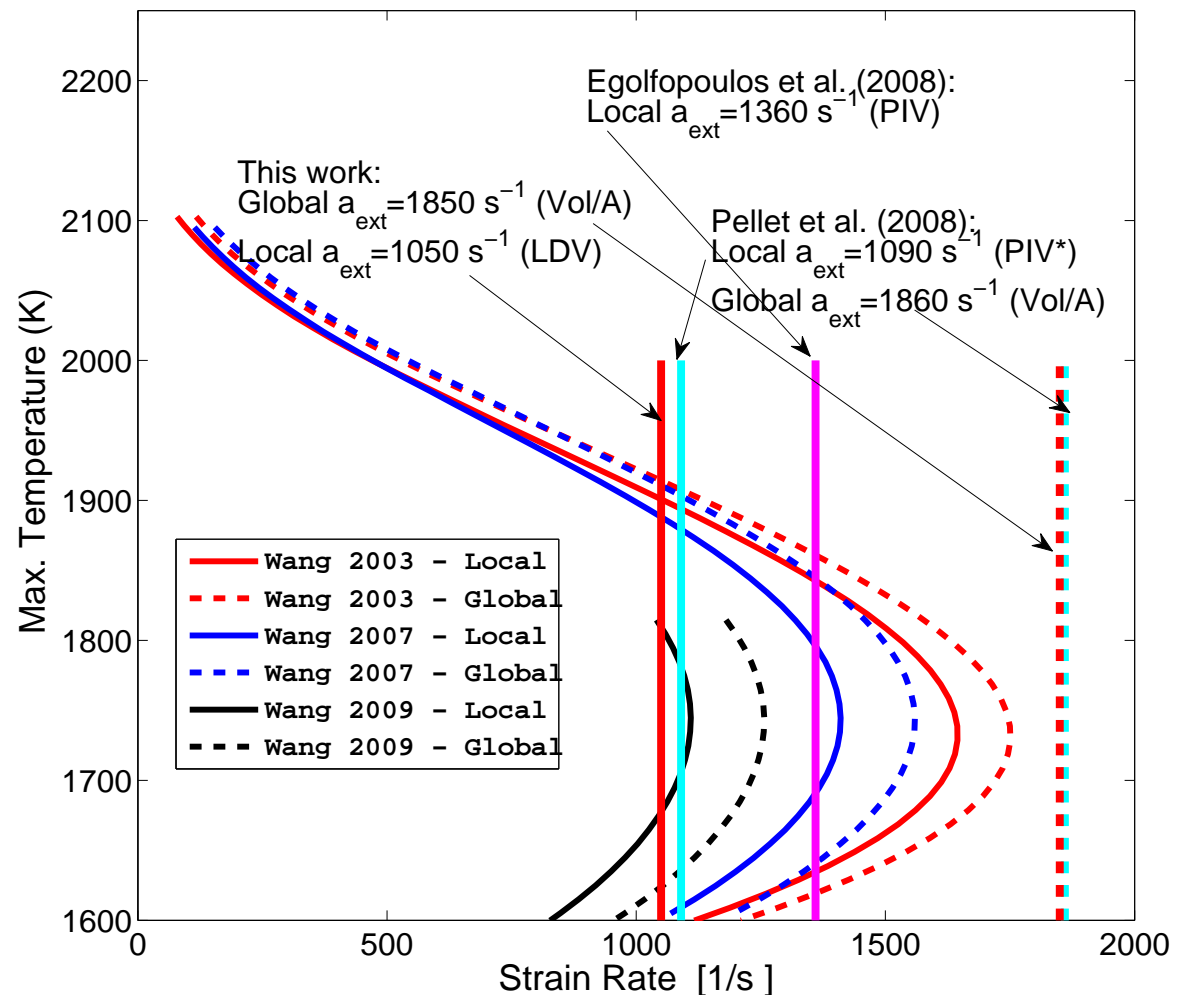
Extinction limit of ethylene-air **Nonpremixed** Flames

- ONE key uncertainty \Rightarrow measurement of strain rate!

- Experiments from USC, NASA Langley, and UVa.

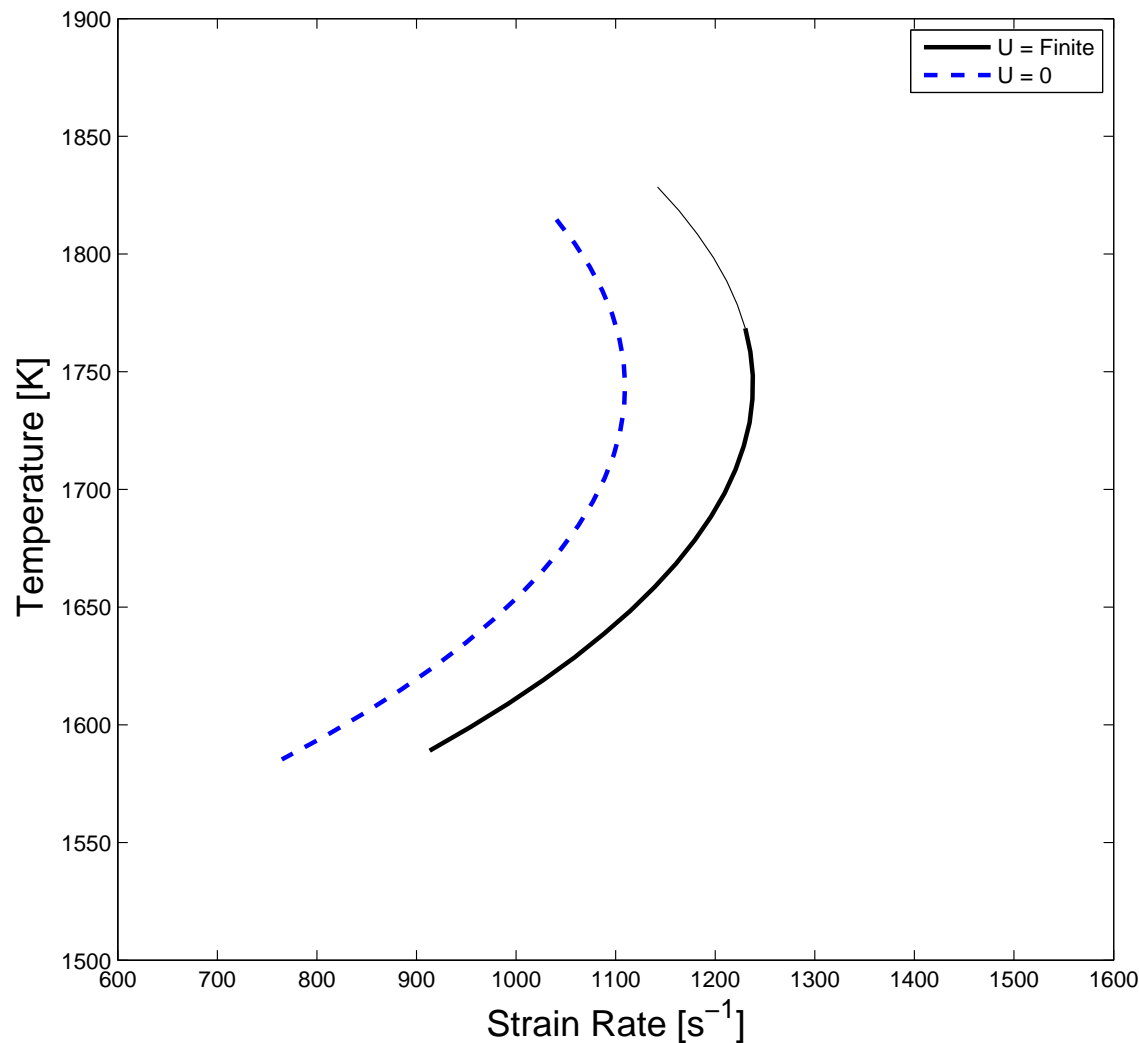
- Chemical kinetic models of Wang and co-workers.

- Full Stefan-Maxwell Eq. to reduce uncertainty of diffusion



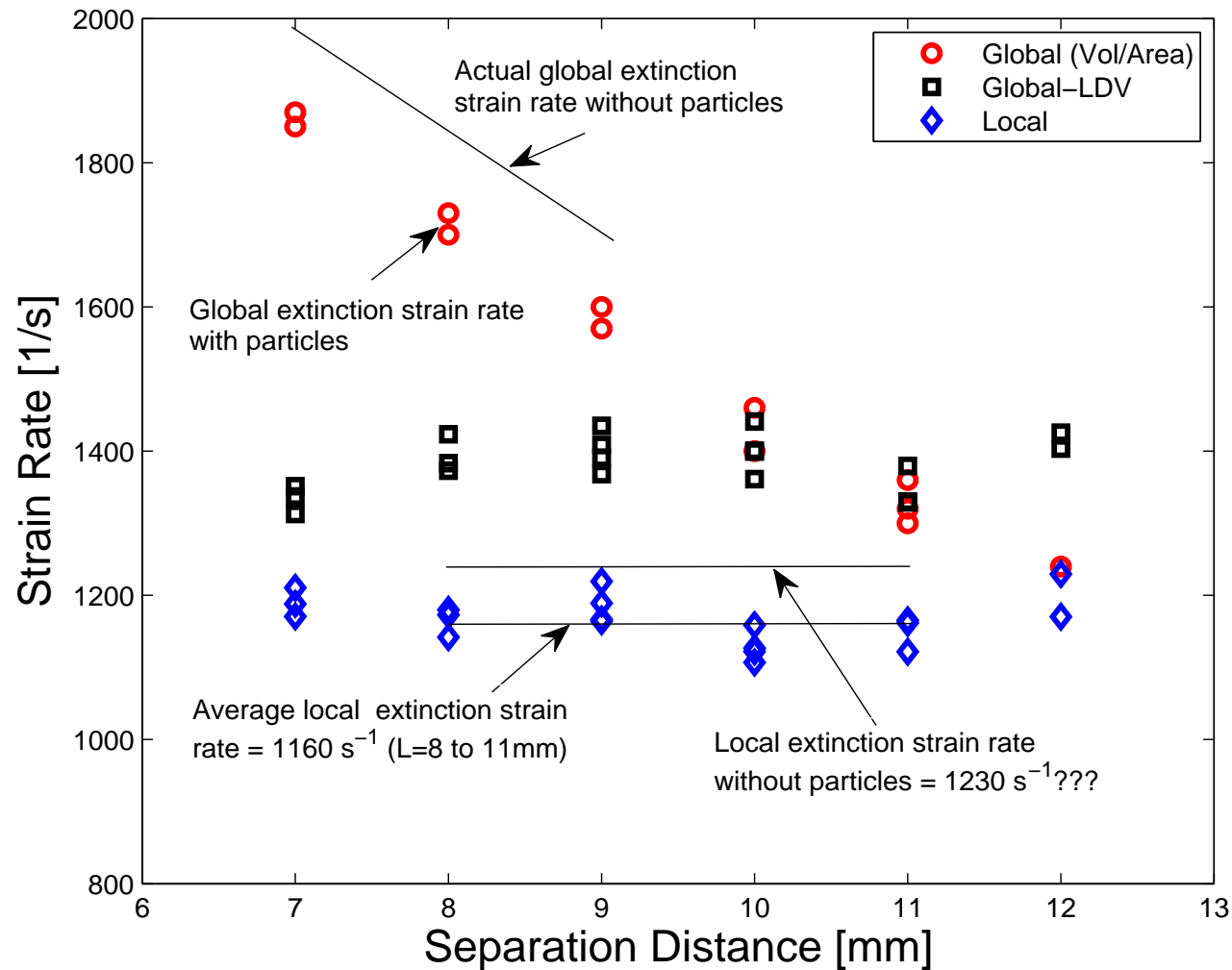
Influence of $U = 0$ vs. $U = \text{Finite}$ on Local Strain Rate

- $dv_z/dz + 2\rho U(z) = 0$ (Kee et al. 1988, Smooke et al., 1990)



Summary of Experimental Data and Uncertainties

- Particle seeding in LDV/PIV \Rightarrow lower local strain rate?

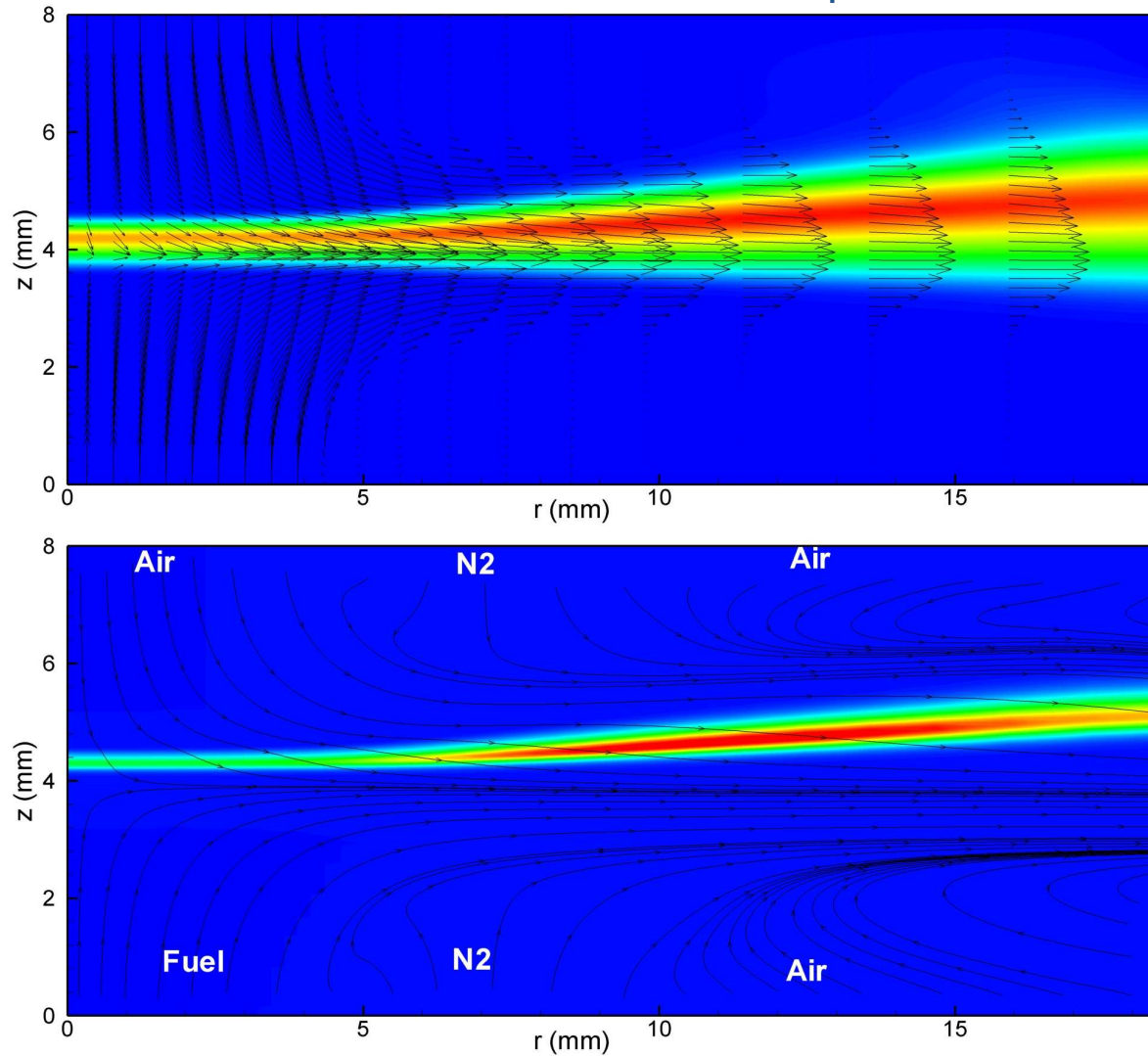


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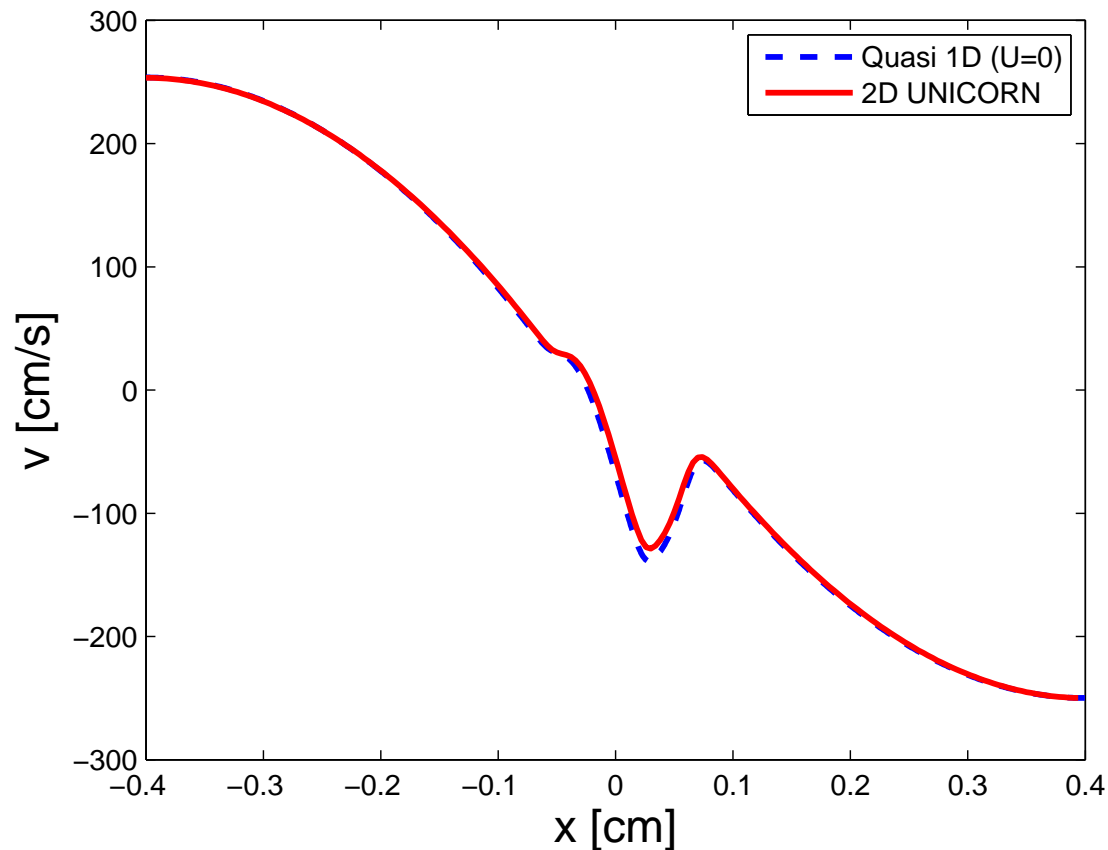
2D Axisymmetric Computations

- Amantini et al. (2007) considered a methane-air case
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Principal Component Analysis with Sensitivity (PCAS)

- Starting point of PCAS is the construction of response function (Vajda, Valko, and Turanyi (1985)):

$$Q(\mathbf{P}) = \sum_{j=1}^q \sum_{i=1}^m \left[\frac{f_i(x_j, \mathbf{P}) - f_i(x_j, \mathbf{P}^0)}{f_i(x_j, \mathbf{P}^0)} \right]^2$$

where \mathbf{P} , \mathbf{P}^0 are unperturbed and perturbed parameters ($k = 1, \dots, p$); f_i a set of target functions ($i = 1, \dots, m$); x_j collection of analysis points ($j = 1, \dots, q$).

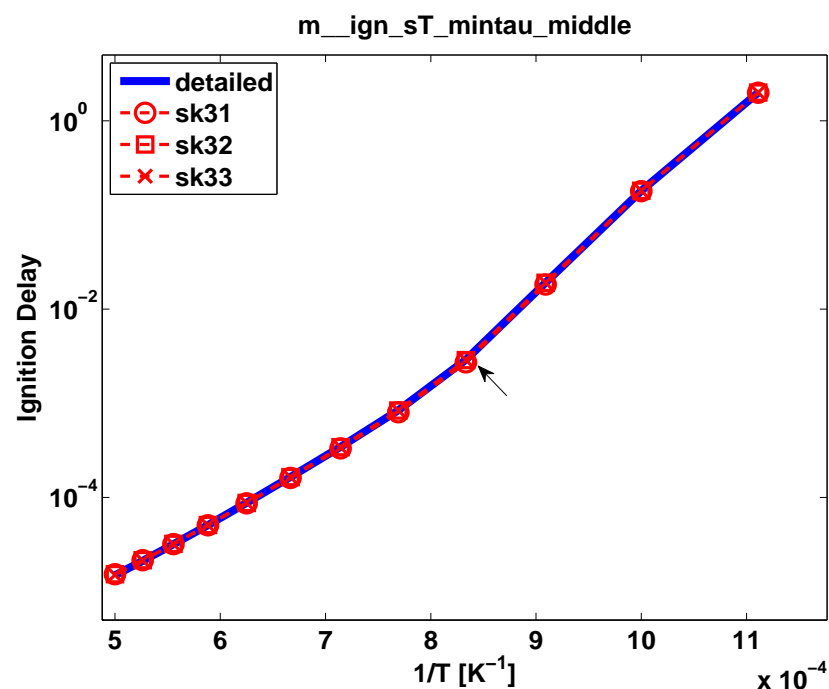
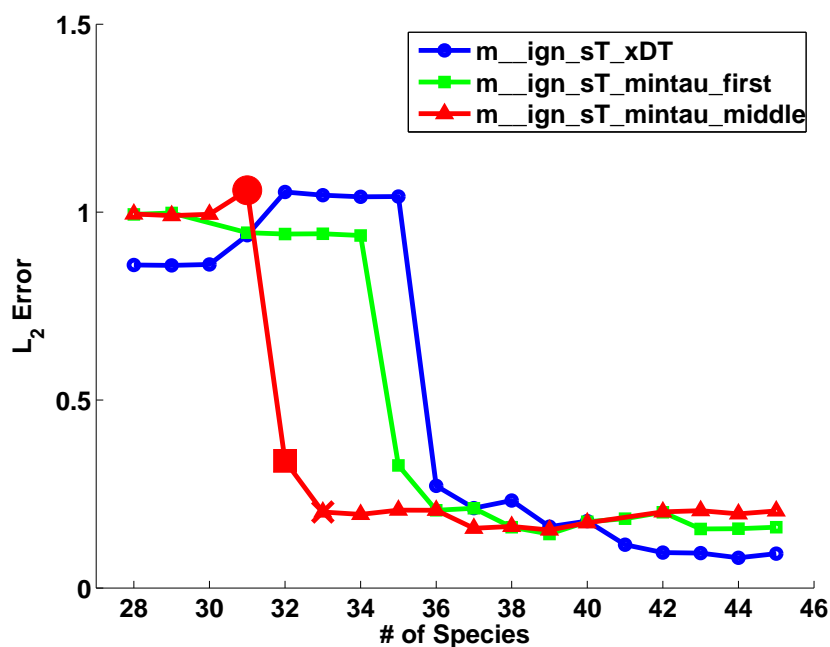
- Around \mathbf{P}^0 , the response function can be approximated as:

$$Q(\mathbf{P}) \approx q(\mathbf{P}) = (\Delta\mathbf{P})^T \mathbf{S}^T \mathbf{S} (\Delta\mathbf{P}) = (\Delta\mathbf{P})^T \mathbf{U}^T \mathbf{\Lambda} \mathbf{U} (\Delta\mathbf{P}) = \sum_{k=1}^p \lambda_k (\Delta\Psi_k)^2$$

where $\Delta\mathbf{P} = \mathbf{P} - \mathbf{P}^0$; \mathbf{S} collection of sensitivity matrices; λ_k eigenvalues; \mathbf{U} normalized eigenvectors; $\Delta\Psi = \mathbf{U}^T \mathbf{P}$ principal components.

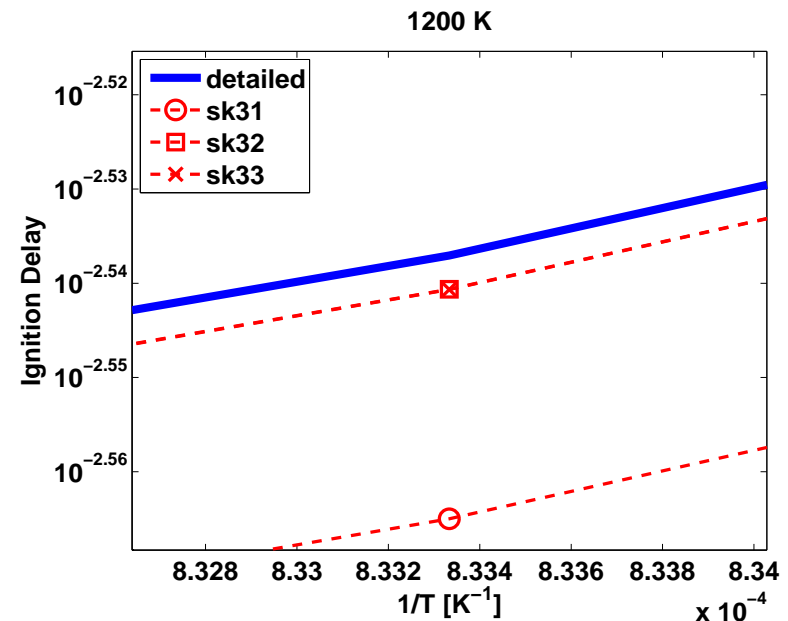
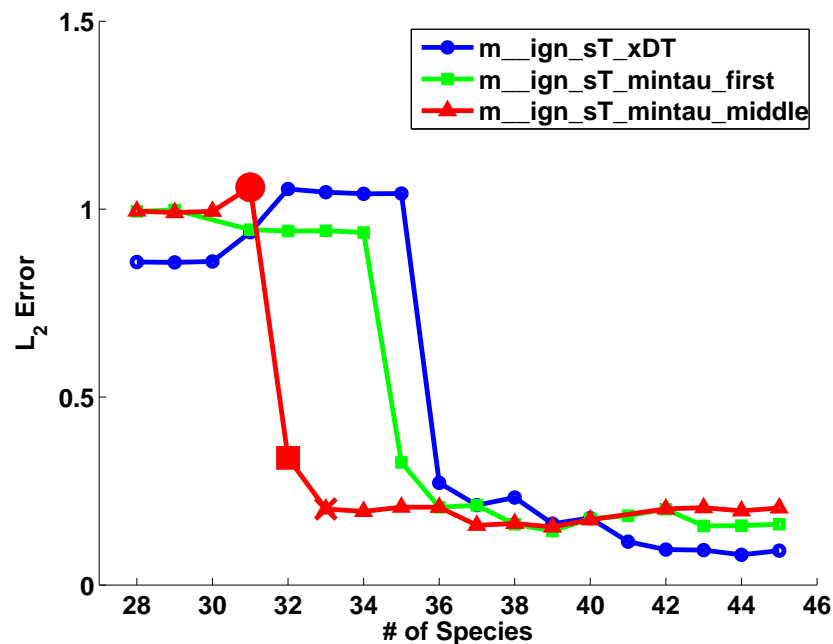
Application of PCAS to Ignition Delay

- Several key issues!!!
- Ethylene-air, $p=1.0\text{atm}$, $\phi=1.0$ with Wang 2003 detailed model (71 species in 467 reactions)



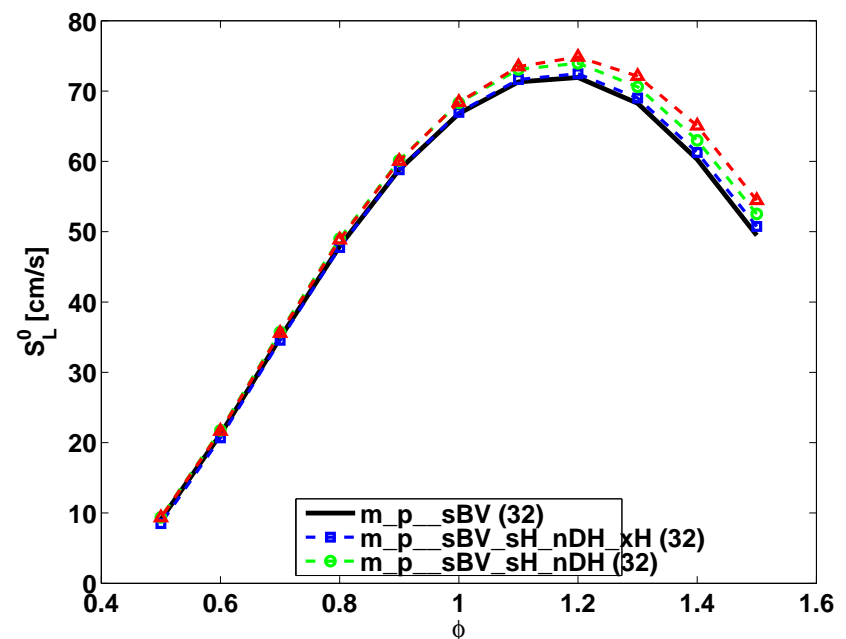
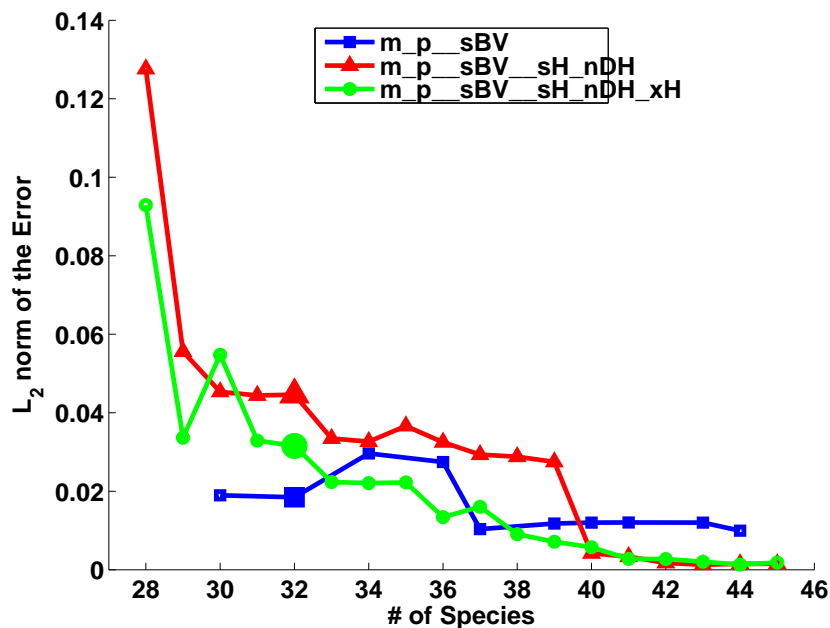
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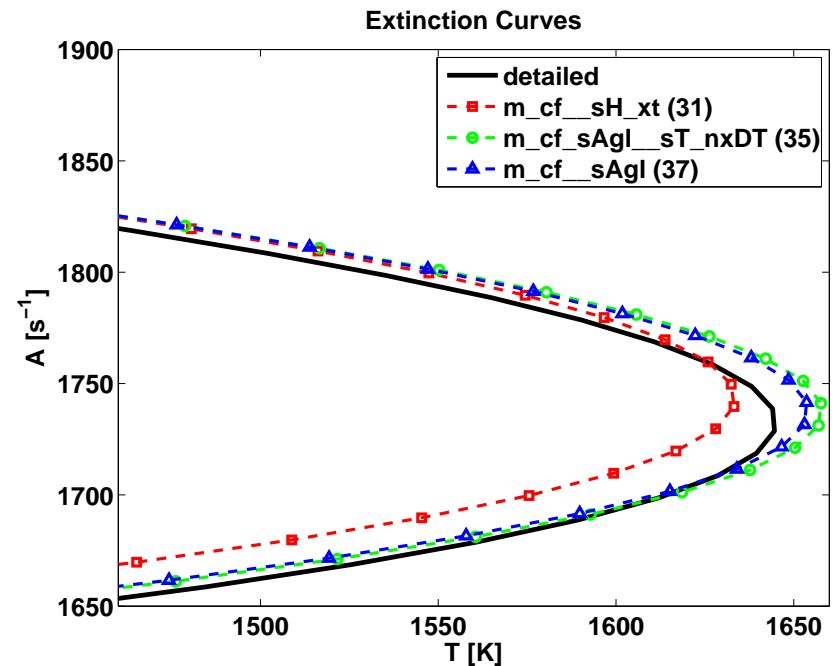
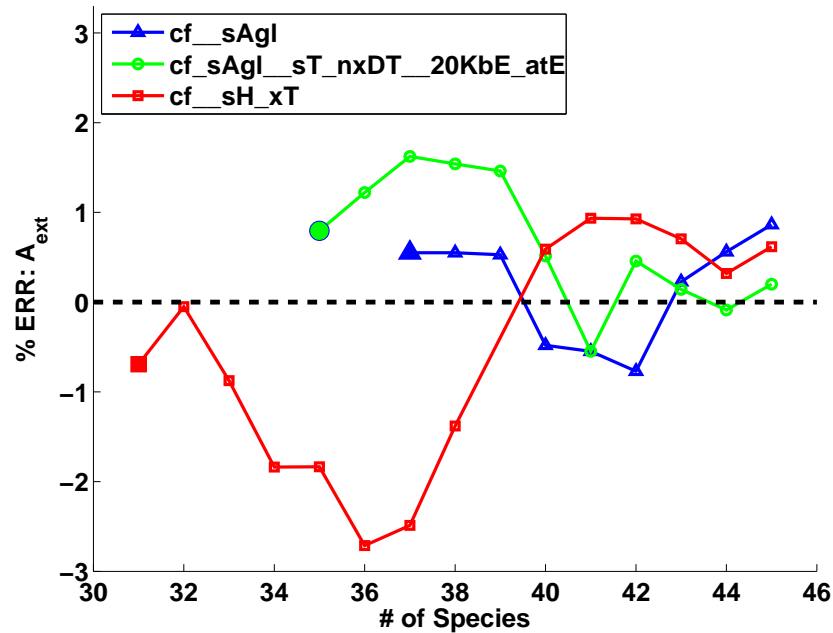
Application of PCAS to Flame Propagation

- Ethylene-air, $p=1.0\text{atm}$, $T_0=300\text{ K}$ with Wang 2003 detailed model (71 species in 467 reactions)



Application of PCAS to Flame Extinction

- Ethylene-air, $p=1.0\text{atm}$, $T_0=300\text{ K}$



QSSA Reduction Approach

- QSSA Reduction Approach — Zambon and Chelliah, *Combustion and Flame* (2007) — 15-step and 18-step reduced reaction models for ethylene-air based on a 31 species and 128 reaction skeletal model from Wang 2003.
- In the process of updating based on USC Mech II Optimized.

NIST Chemical Kinetics Database Program

- Extremely useful tool to analyze differences between chemical kinetic models (Don Burgess)

The screenshot shows the NIST Chemical Kinetics Model Database web interface. The browser address bar displays <http://kinetics.nist.gov/CKMech/ReactionsResults.jsp>. The page header includes the NIST logo and the title "NIST CHEMICAL KINETICS MODEL DATABASE". A navigation bar contains links for OVERVIEW, MODELS, REACTIONS, SPECIES, BIBLIOGRAPHY, and HELP. The user is logged in as Harsha Chelliah, with links for My Bibliography, My Account, and Log Out.

The search results are displayed under the heading "Reaction Search Results". The search criteria are: "Searched for WHERE r.ModelNum=255 and r1.ModelNum=189". The search parameters are: "COMPARING Reactions found in BOTH 2009-Ethylene-Wang AND 2007-C1toC4-Wang", "Written in SAME direction", and "Having DIFFERENT rates with ratio of rate constants > 2.0 over T=800.0-1500.0".

The search results are shown in a table with the following columns: View, Reaction, Class [Sites], log(Ratio), A, b, E, Datatype, Reference, Model, and Kinetics DB. The table displays 5 results, showing the reaction equation, the class of the reaction, the log of the ratio of rate constants, and the pre-exponential factor (A), reaction order (b), and activation energy (E).

View	Reaction	Class [Sites]	log(Ratio)	A	b	E	Datatype	Reference	Model	Kinetics DB
1	$\text{OH} + \text{m} + \text{H} = \text{H}_2\text{O} + \text{m}$	O-H [OH-H] (-)	-0.6	$1.10\text{E}+22$	-2.00	0		2009-Ethylene-Wang		
2	$\text{CH}_3 + (\text{m}) + \text{H} = \text{CH}_4 + (\text{m})$	C-H [CH4] (-)	-0.6	$3.18\text{E}+15$	-0.63	383		2009-Ethylene-Wang		
3	$\text{CH}_3 + \text{OH} = \text{CH}_2\text{-sing} + \text{H}_2\text{O}$	C-H+O [CdH/OH]	-0.7	$1.25\text{E}+14$	0.00	0		2009-Ethylene-Wang	Fwd Rev	
4	$\text{CH}_3 + \text{CH}_3 = \text{C}_2\text{H}_6 + \text{H}$	C-H//C-C (-)	-0.4	$1.41\text{E}+13$	0.10	10600		2009-Ethylene-Wang	Fwd Rev	
5	$\text{C}_2\text{H}_4 + \text{OH} = \text{C}_2\text{H}_5 + \text{H}_2\text{O}$	C-H+O [CdH2/OH]	-0.6	$1.34\text{E}+07$	2.00	2500		2009-Ethylene-Wang	Fwd Rev	

Concluding Remarks

- In quasi 1D extinction limit computations, $U = 0$ and $U = \text{finite}$ (from actual experiments) differ by nearly 10%!!!
- In extinction experiments with convergent nozzles, $L/D = 1$ case shows a non top-hat velocity profile \Rightarrow main contributor to the differences between the measured local strain rate and the global strain rate
- Random errors (1160 ± 20) are too large to extract any systematic uncertainty associated with L/D variation
- detailed reaction models continue to evolve and may converge through collaborative based efforts like PrIME, this Fuels Group, ...
 \Rightarrow need to create **accurate** and **independent** experimental data with well-defined uncertainties
- automated reduction procedures are needed to take advantage of the evolving detailed reaction models (**PCAS/QSSA, ...**)

Acknowledgements

- Hai Wang for sharing kinetic models
- Wing Tsang, Jeff Manion, and Don Burgess at NIST
- OSD T&E and S&T, NASA Hypersonics NRA Program, and AFOSR/NASA National Center for Hypersonic Combined-Cycle Propulsion